Researchers realize highly selective CO hydrogenation to higher alcohols

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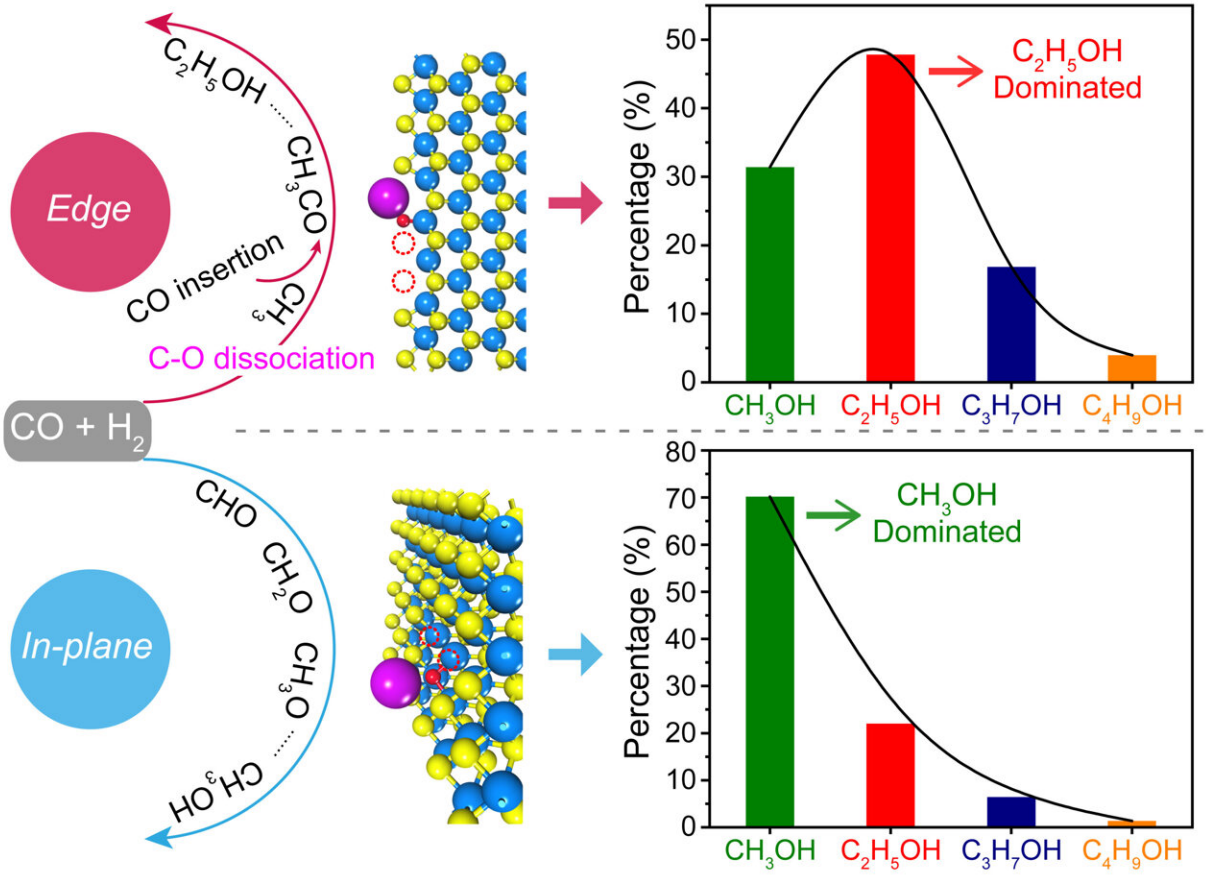

Tunable CO hydrogenation selectivity over MoS_2-based catalyst. Credit: Hu Jingting and Wei Zeyu

Selective hydrogenation of carbon monoxide (CO) to higher alcohols

($C_{2+}OH$) is a promising non-petroleum route for producing high-value chemicals, in which precise regulations of both C-O cleavage and C-C coupling are essential.

Recently, a research group led by Prof. Deng Dehui and Assoc. Prof. Yu Liang from the Dalian Institute of Chemical Physics (DICP) of the Chinese Academy of Sciences (CAS), in collaboration with Prof. Wang Ye from Xiamen University, realized highly selective CO hydrogenation to $C_{2-4}OH$ over a potassium-modified edge-rich molybdenum disulfide (ER-MoS_2-K) catalyst.

This study was published in *Nature Communications* on Oct. 26.

The ER-MoS_2-K catalyst, assembled in nano-array morphology with uniform linear channels, was prepared on the basis of a nano channel-confined growth mechanism.

The researchers found that it could deliver a high CO conversion of 17% with a superior $C_{2-4}OH$ selectivity of 45.2% in hydrogenated products at 240 °C and 50 bar. Moreover, by reducing the lateral size of MoS_2 to enrich edges for boosting carbon-chain growth, the researcher achieved $C_{2-4}OH$ to methanol selectivity ratio overturn from 0.4 to 2.2, and the selectivity of $C_{2-4}OH$ could reach over 99% in $C_{2+}OH$ products.

Sulfur vacancies (SVs) at the edge of MoS_2 boosted carbon-chain growth by facilitating simultaneously the C-O cleavage of CH_xO^* for generating CH_x^* intermediate, and the subsequent C-C coupling between CO* and CH_x^*, while the potassium promoter promoted the desorption of alcohols via electrostatic interaction with hydroxyls, thereby enabling controllable formation of $C_{2-4}OH$.

"Our work presents the high flexibility of edge SVs of MoS_2 in tailoring both C-O cleavage and C-C coupling for carbon-chain growth in CO

hydrogenation, thus providing a prototype for the rational design of nanostructure and microenvironment of active sites for selective hydrogenation reactions," said Prof. Deng.

More information: Jingting Hu et al, Edge-rich molybdenum disulfide tailors carbon-chain growth for selective hydrogenation of carbon monoxide to higher alcohols, *Nature Communications* (2023). DOI: 10.1038/s41467-023-42325-z

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